Machine Learning–Enhanced Life Cycle Assessment for Predictive Sustainability Optimization Across Industrial, Agricultural, and Built Environments

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Abstract

The accelerating urgency of climate change, resource depletion, and ecological degradation has placed unprecedented pressure on industries, governments, and researchers to adopt more reliable, forward-looking, and operationally relevant sustainability assessment tools. Life cycle assessment (LCA), standardized through ISO 14044, has long served as the methodological backbone for evaluating environmental impacts across product and process life cycles, yet its traditional reliance on static inventories, linear modeling assumptions, and data-intensive workflows has increasingly limited its ability to address complex, rapidly evolving technological systems (ISO, 2006). In parallel, machine learning and artificial intelligence have emerged as transformative analytical paradigms capable of discovering nonlinear relationships, filling data gaps, forecasting future conditions, and optimizing multi-objective systems. The convergence of these two domains represents a fundamental methodological transition from retrospective and descriptive environmental accounting toward predictive, adaptive, and decision-oriented sustainability science.

This article develops a comprehensive theoretical and empirical synthesis of machine learning–integrated life cycle assessment based strictly on the scientific foundations provided by the referenced literature. Drawing on studies spanning construction materials, buildings, energy systems, agriculture, transportation, chemical processes, and emerging biotechnologies, the paper demonstrates how artificial intelligence is reshaping every phase of the LCA workflow, including inventory generation, impact factor estimation, uncertainty modeling, scenario forecasting, and optimization of sustainability trade-offs (Dabbaghi et al., 2021; Ghoroghi et al., 2022; Kock et al., 2023; Kleinekorte et al., 2023). Unlike conventional LCA approaches that depend on historical averages and fixed system boundaries, machine learning–enabled frameworks are shown to operate as dynamic, learning-based representations of socio-technical systems that evolve as new data, technologies, and climate conditions emerge.

The article further explains how predictive modeling, surrogate process modeling, deep neural networks, fuzzy systems, genetic algorithms, and reinforcement learning collectively allow LCA to move from ex-post environmental auditing to ex-ante sustainability design (Karka et al., 2022; Huntington et al., 2023; Kazemeini and Swei, 2023). Empirical evidence from sectors such as concrete production, bioenergy, crop cultivation, vehicle manufacturing, and carbon capture illustrates that AI-enhanced LCA can drastically improve both accuracy and decision relevance by capturing nonlinear process behavior, regional variability, and long-term uncertainty (Kaab et al., 2019; Lee et al., 2020; Javadi et al., 2021; Dong and Zhang, 2023). Importantly, the study also interrogates the epistemological and governance implications of embedding learning algorithms within environmental accounting systems, addressing issues of transparency, data bias, reproducibility, and policy legitimacy.

By synthesizing theoretical developments, methodological innovations, and sector-specific applications, this article establishes a unified conceptual framework for intelligent life cycle assessment. It argues that machine learning is not merely a computational enhancement but a paradigm shift that transforms sustainability assessment into a predictive, optimization-driven, and policy-relevant discipline capable of guiding the global transition toward low-carbon and resource-efficient societies.

Keywords: Life cycle assessment, machine learning, environmental sustainability, carbon footprint, predictive modeling, eco-design, energy systems

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1. Introduction

The Life cycle assessment has evolved over the past several decades into the most widely accepted methodological framework for quantifying the environmental impacts associated with products, processes, and services across their entire life cycles, from raw material extraction through production, use, and end-of-life treatment. The standardization of LCA under ISO 14044 provided a formalized structure for defining system boundaries, compiling inventories, conducting impact assessment, and interpreting results in a transparent and comparable way (ISO, 2006). This standardization was a critical milestone in transforming sustainability from a qualitative aspiration into a quantitative decision-making framework, enabling governments and industries to compare technological options, set regulatory thresholds, and design environmental policies. However, the very features that gave LCA its rigor—fixed inventories, deterministic modeling, and static assumptions—have increasingly become sources of limitation as global systems grow more complex, data-rich, and uncertain.

Modern production systems are no longer characterized by stable technologies and predictable supply chains. They are dynamic, multi-scale, and deeply interconnected with climatic, economic, and social processes. Buildings change their energy performance over decades, crops respond to evolving climate conditions, and industrial processes are continuously redesigned to incorporate new materials and energy sources (Ji et al., 2021; Lee et al., 2020; Dong and Zhang, 2023). Traditional LCA, which relies heavily on historical averages and generic databases, struggles to capture these dynamics, often producing results that are backward-looking rather than decision-relevant for future-oriented sustainability planning. Moreover, the compilation of life cycle inventories remains one of the most resource-intensive and uncertain steps in LCA, with data gaps, inconsistent reporting, and regional variability introducing large uncertainties that propagate through impact results (Khadem et al., 2022; Kock et al., 2023).

At the same time, the digitalization of industrial systems, the proliferation of sensors, and the expansion of computational power have generated unprecedented volumes of data describing material flows, energy use, emissions, and process behavior. Machine learning and artificial intelligence have emerged precisely to address the challenges posed by such complex, high-dimensional data environments. By learning patterns directly from data rather than relying on predefined equations, machine learning models can capture nonlinear relationships, identify hidden drivers of environmental performance, and generate reliable predictions even in the presence of incomplete information (Ghoroghi et al., 2022; Huntington et al., 2023).

The integration of machine learning into life cycle assessment therefore represents a structural transformation of sustainability science. Instead of treating environmental impacts as static outputs derived from fixed inputs, AI-enabled LCA frameworks treat sustainability as a dynamic system that can be learned, forecasted, and optimized. Studies have already demonstrated that artificial neural networks can predict energy use and environmental impacts of buildings more accurately than conventional engineering models (D'Amico et al., 2019), that deep belief networks can optimize the life cycle performance of concrete mixtures (Dabbaghi et al., 2021), and that machine learning can project national building-sector carbon footprints decades into the future (Dong and Zhang, 2023). In agriculture, AI-based models have been used to predict crop yields and greenhouse gas emissions simultaneously, enabling the optimization of water, energy, and fertilizer use within a life cycle framework (Kaab et al., 2019; Nabavi-Pelesaraei et al., 2020).

Despite this growing body of research, the conceptual foundations of machine learning–integrated LCA remain fragmented. Many studies focus on specific applications, such as a single crop, a particular material, or one industrial process, without situating these advances within a broader theoretical framework. Moreover, the implications of embedding learning algorithms into environmental accounting systems for transparency, policy credibility, and ethical governance are rarely examined in depth. There remains a significant gap between the technical promise of AI and the institutional structures that govern sustainability decision-making.

This article addresses that gap by synthesizing the referenced literature into a unified analytical framework that explains how machine learning is reshaping the epistemology, methodology, and practice of life cycle assessment. By examining how AI techniques are applied to inventory modeling, impact factor estimation, scenario forecasting, and multi-objective optimization across diverse sectors, the paper demonstrates that intelligent LCA constitutes a new generation of sustainability science. This new generation is characterized not by static snapshots of environmental performance, but by adaptive, predictive, and decision-support-oriented representations of complex socio-technical systems.

2. Methodology

The methodological foundation of this research article is built upon a structured theoretical synthesis of the referenced scientific literature, combined with a conceptual integration of machine learning and life cycle assessment frameworks. In accordance with ISO 14044, LCA consists of four interrelated phases: goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and interpretation (ISO, 2006). The methodological innovation examined in this study lies in the transformation of each of these phases through the incorporation of artificial intelligence techniques.

The first methodological dimension concerns the generation and refinement of life cycle inventory data. Traditional LCI compilation relies on process-based measurements, industrial surveys, and secondary databases. However, such data are often incomplete, inconsistent, or unavailable for emerging technologies and regionalized systems. Machine learning provides a statistical and computational framework for inferring missing data, interpolating between sparse observations, and predicting process flows under new conditions. Feed-forward neural networks, deep belief networks, and surrogate models have been used to predict energy use, emissions, and material flows in manufacturing, agriculture, and chemical processes with high accuracy (Dabbaghi et al., 2021; Khadem et al., 2022; Huntington et al., 2023). These models learn from historical process data and can generalize to new parameter combinations, enabling the construction of dynamic inventories that evolve as system inputs change.

A second methodological pillar is the estimation of characterization factors and impact categories. In conventional LCA, impact factors such as global warming potential or ecotoxicity are derived from complex physical and chemical models that require extensive experimental data. Machine learning has been applied to estimate these factors directly from molecular descriptors, environmental fate data, and observed toxicity outcomes, greatly expanding the scope and resolution of impact assessment (Hou et al., 2020). By learning relationships between chemical properties and environmental behavior, AI-based models allow LCA to include substances and processes that would otherwise remain outside the analytical boundary.

The third methodological dimension involves scenario modeling and forecasting. Sustainability decisions are inherently future-oriented, yet traditional LCA is fundamentally retrospective, based on historical averages. Machine learning enables the projection of life cycle impacts under future climate, technology, and policy scenarios by learning from time-series data and climate models. Studies on building-sector carbon footprints and agricultural systems demonstrate that AI can simulate how emissions trajectories respond to evolving energy mixes, climate conditions, and technological adoption (Lee et al., 2020; Dong and Zhang, 2023). These predictive capabilities transform LCA into a strategic planning tool rather than merely an accounting framework.

The fourth methodological dimension concerns optimization and decision support. Sustainability problems are typically multi-objective, involving trade-offs between cost, energy use, greenhouse gas emissions, water consumption, and ecological impacts. Metaheuristic algorithms, genetic algorithms, and reinforcement learning have been integrated with LCA models to identify optimal configurations of resources, technologies, and management strategies (Kaab et al., 2019; Karamian et al., 2023; Kazemeini and Swei, 2023). These techniques search large solution spaces to find Pareto-optimal solutions that balance competing sustainability goals.

Throughout the article, these methodological components are not treated as isolated techniques but as elements of a coherent intelligent LCA framework. This framework conceptualizes sustainability assessment as a learning-based system that continuously updates its representations of environmental performance as new data, technologies, and policies emerge.

3. Results

The integration of machine learning into life cycle assessment has generated a wide array of empirical outcomes across multiple sectors, consistently demonstrating improvements in accuracy, predictive power, and decision relevance. In the domain of construction materials, Dabbaghi et al. (2021) showed that deep belief networks combined with multi-objective optimization could identify lightweight aggregate concrete mixtures that minimize both environmental impacts and material costs. By learning from experimental data on material composition and performance, the model was able to explore a vast design space that would be infeasible using conventional trial-and-error or linear regression approaches. The resulting optimized mixtures exhibited significantly lower embodied carbon and energy use compared to traditional formulations, illustrating how AI-driven LCA can guide eco-design at the material level.

In the built environment, artificial neural networks have been used to assess and forecast the energy and environmental performance of buildings. D'Amico et al. (2019) demonstrated that neural networks trained on Italian building data could predict life cycle energy consumption and emissions more accurately than conventional simulation tools. Building lifespan prediction, a critical parameter in LCA and life cycle costing, has also been enhanced through machine learning applied to large datasets of building characteristics and performance histories (Ji et al., 2021). These predictive models reduce uncertainty in long-term impact estimates, which is particularly important for infrastructure investments with lifespans of several decades.

At the urban and national scale, machine learning has enabled the projection of carbon footprints under future scenarios. Dong and Zhang (2023) used machine learning to forecast Hong Kong's building-sector emissions through 2050, accounting for changes in energy systems, technology adoption, and economic growth. Such forward-looking assessments provide policymakers with quantitative insights into the feasibility of carbon neutrality targets, something traditional LCA frameworks are not designed to do.

In agriculture, AI-integrated LCA has produced particularly rich results due to the highly variable and data-intensive nature of farming systems. Neural networks, fuzzy inference systems, and genetic algorithms have been used to predict crop yields, energy use, and greenhouse gas emissions simultaneously, enabling the optimization of cropping systems within a life cycle framework (Khanali et al., 2017; Khoshnevisan et al., 2014; Nabavi-Pelesaraei et al., 2020). These models capture the nonlinear interactions between weather, soil conditions, input use, and management practices, providing farmers and policymakers with actionable sustainability metrics that reflect real-world variability.

In energy and industrial systems, machine learning has been used to generate surrogate models of complex processes, enabling rapid evaluation of environmental impacts without the need for full-scale process simulation. Huntington et al. (2023) demonstrated that machine learning could accurately approximate the life cycle performance of bioproduction pathways, while Liao et al. (2020) used AI to generate energy and greenhouse gas inventories for activated carbon production. These surrogate models make it possible to screen large numbers of technological alternatives early in the design process, accelerating innovation while maintaining environmental accountability.

Across all these domains, a consistent result emerges: machine learning reduces data gaps, captures system complexity, and provides predictive insights that fundamentally enhance the usefulness of life cycle assessment for sustainability decision-making.

4. Discussion

The empirical successes of machine learning–integrated life cycle assessment reflect deeper theoretical transformations in how environmental knowledge is produced and used. Traditional LCA is grounded in a mechanistic epistemology, where environmental impacts are calculated through predefined causal chains linking inputs, processes, and emissions. While this approach ensures transparency and interpretability, it struggles with complexity, uncertainty, and novelty. Machine learning introduces a data-driven epistemology in which relationships are inferred from observed patterns rather than imposed by theory. This shift allows LCA to handle nonlinear dynamics, high-dimensional interactions, and evolving technologies, but it also raises important questions about explainability, trust, and governance.

One of the central advantages of AI-based LCA is its ability to operate under uncertainty. Climate change, technological innovation, and economic volatility mean that future environmental impacts cannot be reliably inferred from past averages. By learning from time-series data and scenario inputs, machine learning models can generate probabilistic forecasts that reflect a range of possible futures (Lee et al., 2020; Dong and Zhang, 2023). This aligns LCA with the needs of strategic planning and risk management, transforming it from a descriptive tool into a predictive one.

At the same time, the use of black-box models challenges the traditional transparency of LCA. Regulatory frameworks and environmental labeling schemes rely on traceable and auditable calculations. When neural networks or ensemble models generate impact estimates, the causal pathways may be opaque, potentially undermining trust. This tension has led to the development of hybrid approaches that combine mechanistic LCA models with machine learning surrogates, preserving interpretability while enhancing predictive performance (Karka et al., 2022; Kleinekorte et al., 2023).

Another critical issue is data bias and representativeness. Machine learning models are only as good as the data on which they are trained. If training datasets are skewed toward certain regions, technologies, or scales of operation, the resulting predictions may systematically misrepresent environmental performance elsewhere. This is particularly important in global sustainability assessments, where data from industrialized regions often dominate (Ghoroghi et al., 2022). Addressing this challenge requires coordinated efforts to expand and harmonize environmental data infrastructures.

The integration of optimization algorithms further complicates the ethical and political dimensions of sustainability assessment. When genetic algorithms or reinforcement learning identify optimal strategies for reducing emissions or resource use, they implicitly encode value judgments about trade-offs between economic, environmental, and social objectives (Kaab et al., 2019; Kazemeini and Swei, 2023). Making these value assumptions explicit is essential for democratic accountability in sustainability policy.

5. Conclusion

The convergence of machine learning and life cycle assessment marks a profound transformation in the science and practice of sustainability. By enabling dynamic inventory modeling, predictive impact assessment, and multi-objective optimization, artificial intelligence allows LCA to move beyond retrospective accounting toward proactive sustainability design. The referenced literature demonstrates that across construction, agriculture, energy, transportation, and chemical industries, AI-enhanced LCA delivers more accurate, more relevant, and more actionable insights than conventional approaches.

Yet this transformation also introduces new challenges of transparency, data governance, and ethical decision-making. The future of intelligent LCA will depend not only on advances in algorithms but also on the development of institutional frameworks that ensure that these powerful tools are used responsibly, equitably, and in service of genuine sustainability transitions. When combined with the rigor of ISO-based LCA and the adaptive intelligence of machine learning, environmental assessment can become a cornerstone of a data-driven, climate-resilient global economy.

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